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| Title: | Advancing a phase field dislocation dynamics code to model HCP materials |
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# Advancing a phase field dislocation dynamics code to model HCP materials


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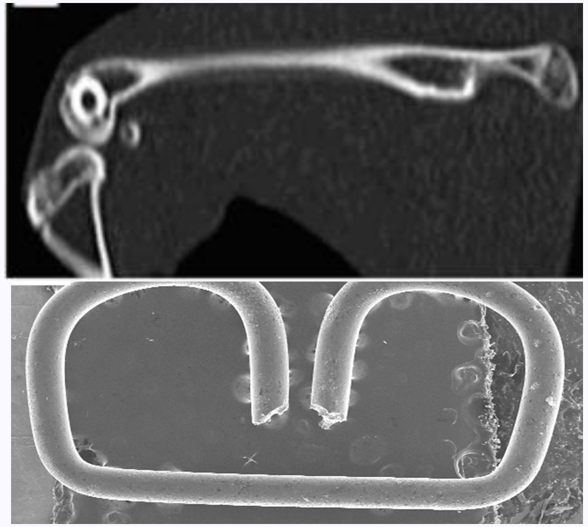
[4] T-3: Fluid Dynamics and Solid Mechanics
[5] MST-8: Materials Science in Radiation & Dynamics Extremes

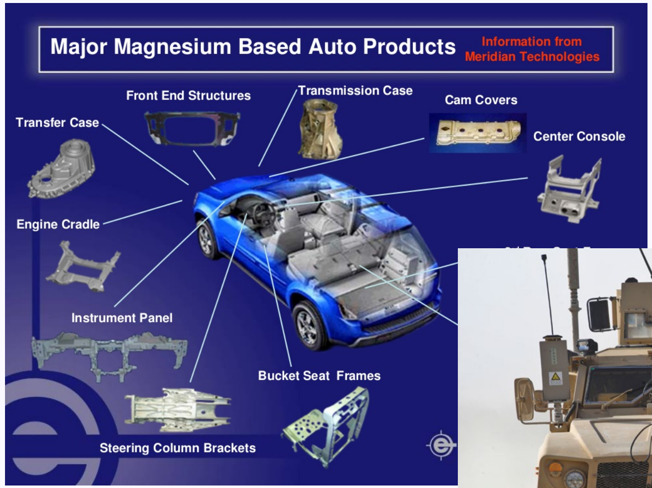
# Motivation: HCP metals and their alloys

- High strength to weight ratio, biocompatibility, radiation resistance, fatigue resistance

Biomedical



Automotive




Aerospace



# Phase Field Dislocation Dynamics **PFDD** Model

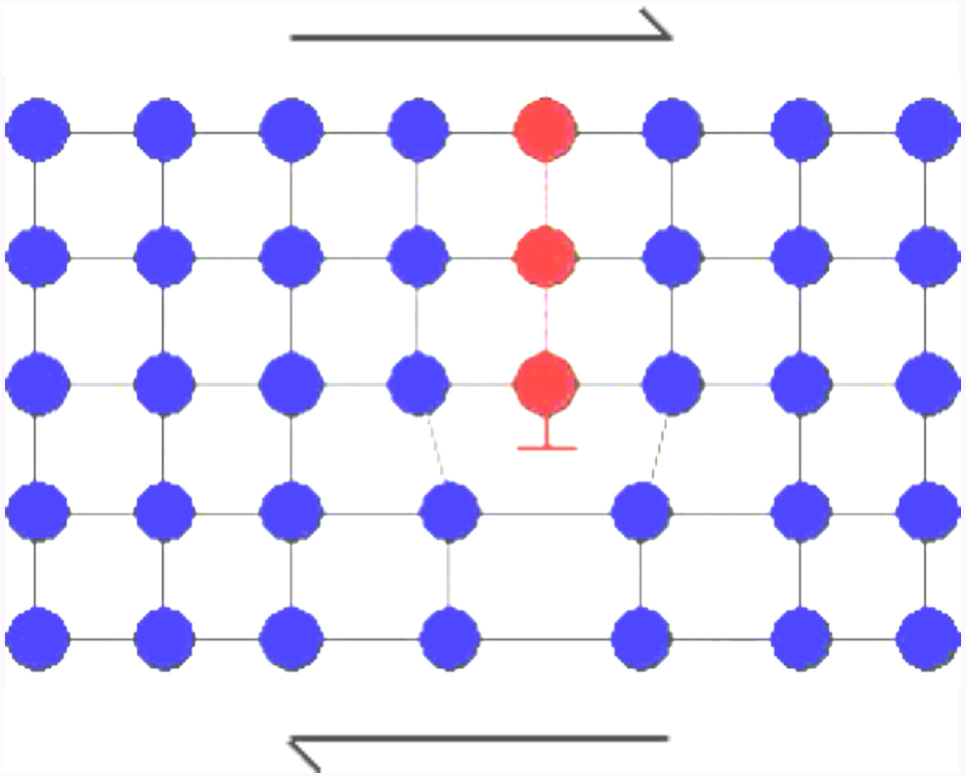
- Phase field frameworks describe physical behavior by tracking one or more **scalar order parameters** $(\zeta)$ and evolving them through the **minimization of the system's total energy** $(\mathbf{E})$, equilibrating between every time step.

$$\frac{\delta E(\zeta)}{\delta \zeta} = 0$$

$$E = E^{strain} + E^{\,core}$$

- When a dislocation slips the atoms change neighbors and the order parameter takes on a value of 1. The order parameter remains 0 if no slip occurs.

**Perfect Edge Dislocation Movement**



www.youtube.com/watch?v=iKKxTP6xp74

$$\epsilon_{ij}^{p}(\boldsymbol{x},t) = \frac{1}{2}\sum_{\alpha=1}^{N} b\zeta_{\alpha}(\boldsymbol{x},t)\delta_{n}(s_i^{\alpha}m_j^{\alpha} + s_j^{\alpha}m_i^{\alpha})$$

- **Plasticity** or deformation is mediated by the motion and interaction of dislocations
- Thus the **plastic strain**, $\epsilon_{ij}^{p}(\boldsymbol{x},t)$, will be directly proportional to the number of gliding dislocations which are our phase field variable, $\zeta$ (order parameter).

N = number of slip systems

α = a specific slip system

$s^{\alpha}$ = slip direction

$m^{\alpha}$ = normal to the slip plane

$\delta_n$ = Dirac distribution supported on the slip plane, n

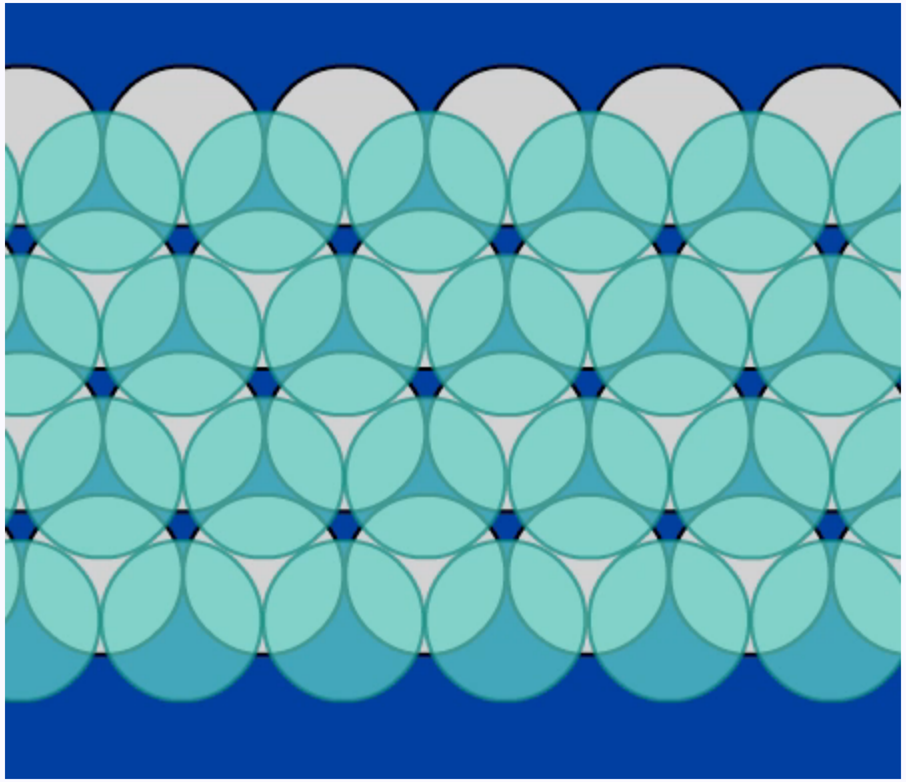
b = the magnitude of the Burgers vector

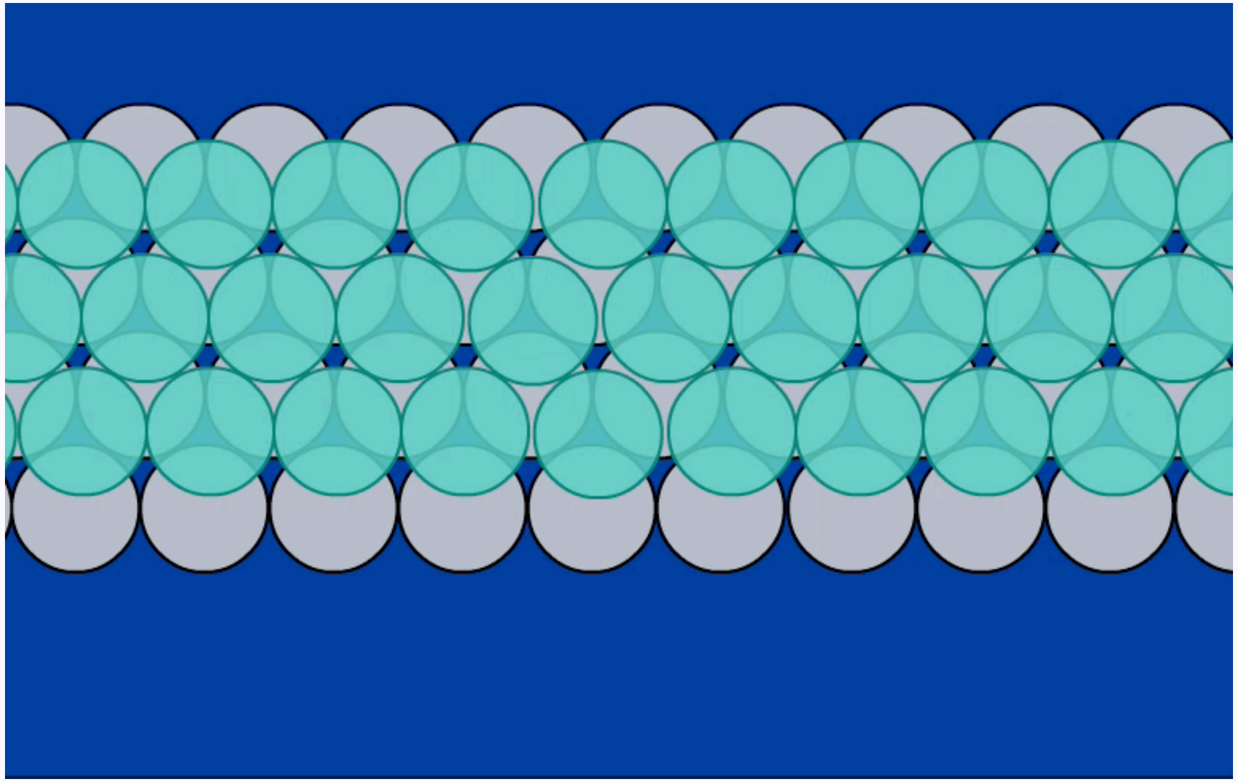
$$\hat{A}_{mnuv}(\boldsymbol{k}) = C_{mnuv} - C_{kluv}C_{ijmn}\hat{G}_{ki}(k)k_j k_l$$

$$E^{strain}(\zeta) = \frac{1}{2}\int \hat{A}_{mnuv}(\boldsymbol{k})\hat{\epsilon}_{mn}^{p}(\boldsymbol{k})\hat{\epsilon}_{mn}^{p*}(\boldsymbol{k})\frac{d^3k}{(2\pi)^3} - \int \sigma_{ij}^{appl}\epsilon_{ij}^{p}\, d^3x$$

# Partial dislocations & stacking fault widths

It is energetically favorable for a perfect dislocation to split into two **partial dislocations**. These two partials are like signed and repel each other, generating a **stacking fault width**.

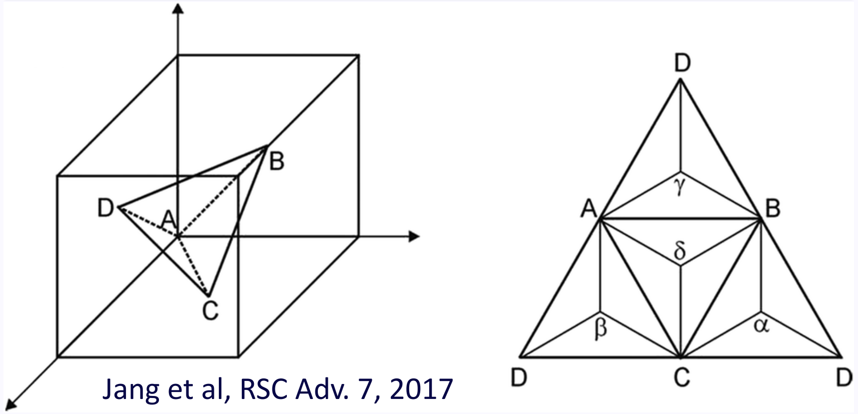




www.princeton.edu/~maelabs/mae324/07/07mae_52a.htm

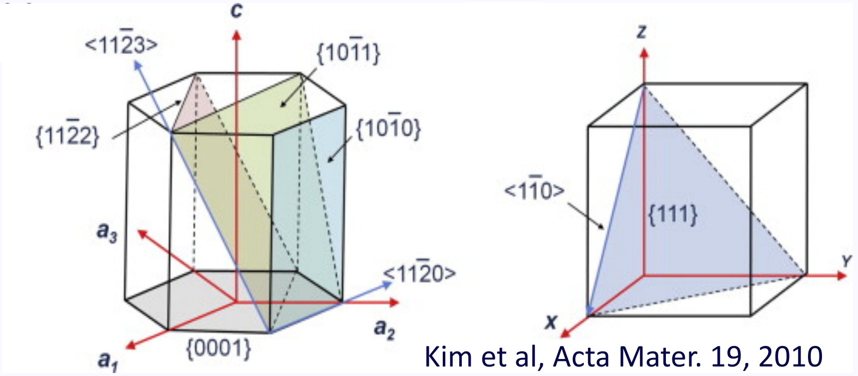
# Face Centered Cubic & Hexagonal Close Packed

## Thompson Tetrahedron



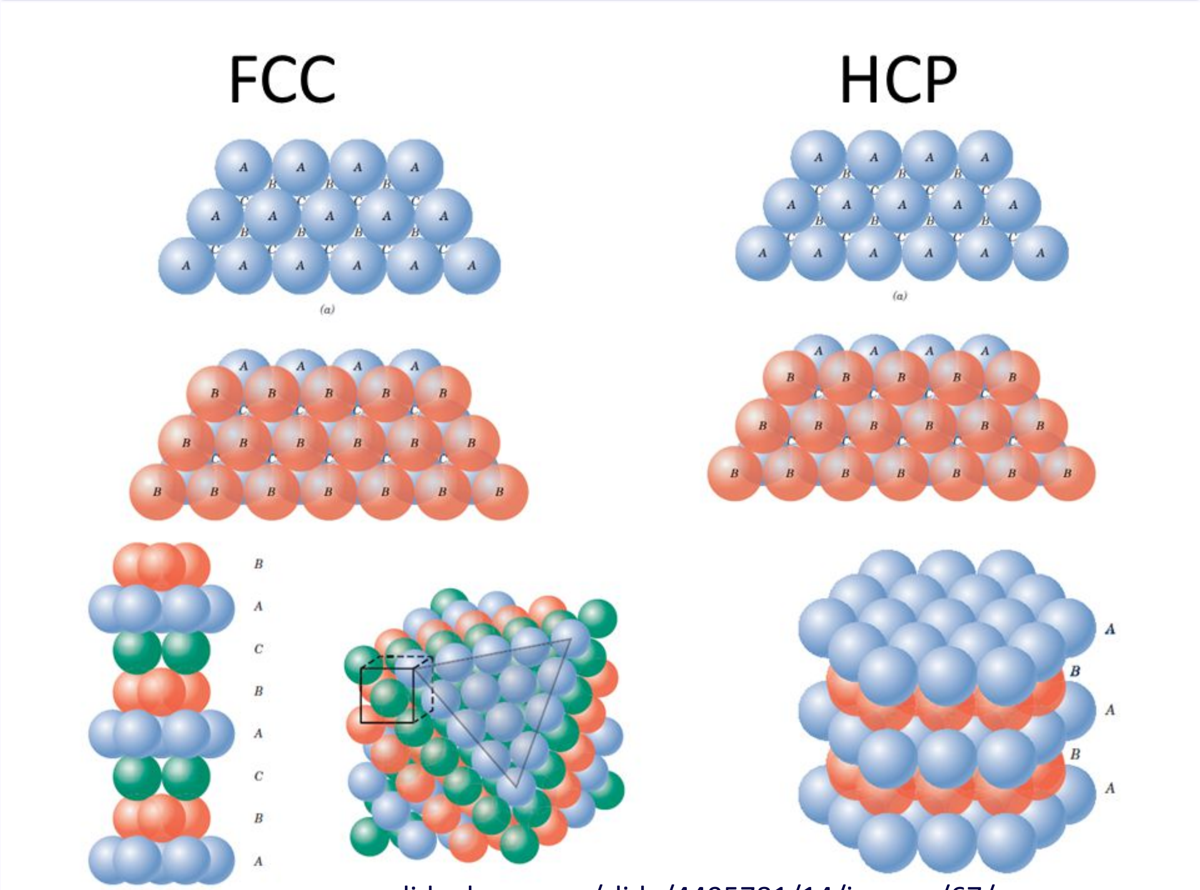

Jang et al, RSC Adv. 7, 2017

## Slip Planes




Kim et al, Acta Mater. 19, 2010

## {111} in FCC vs {0001} in HCP

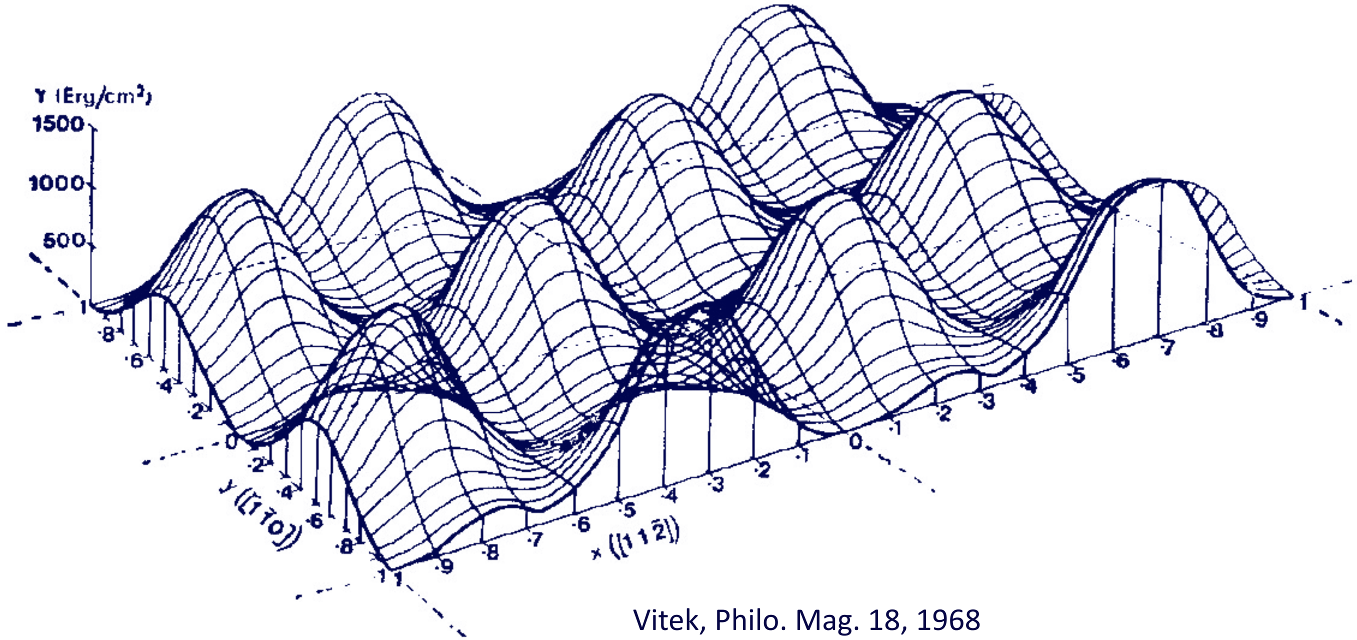



slideplayer.com/slide/4495781/14/images/67/

# Core energy and γ-surface

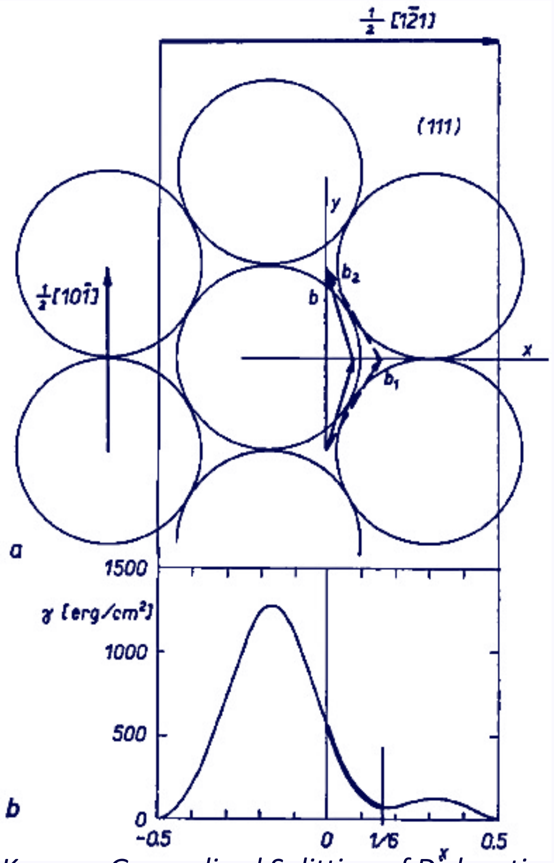
## Perfect Dislocations

$$E^{core}(\zeta) = \sum_{\alpha=1}^{N} \int B sin^2(n\pi\zeta_\alpha(\boldsymbol{x}, t))\delta_n d^3x$$



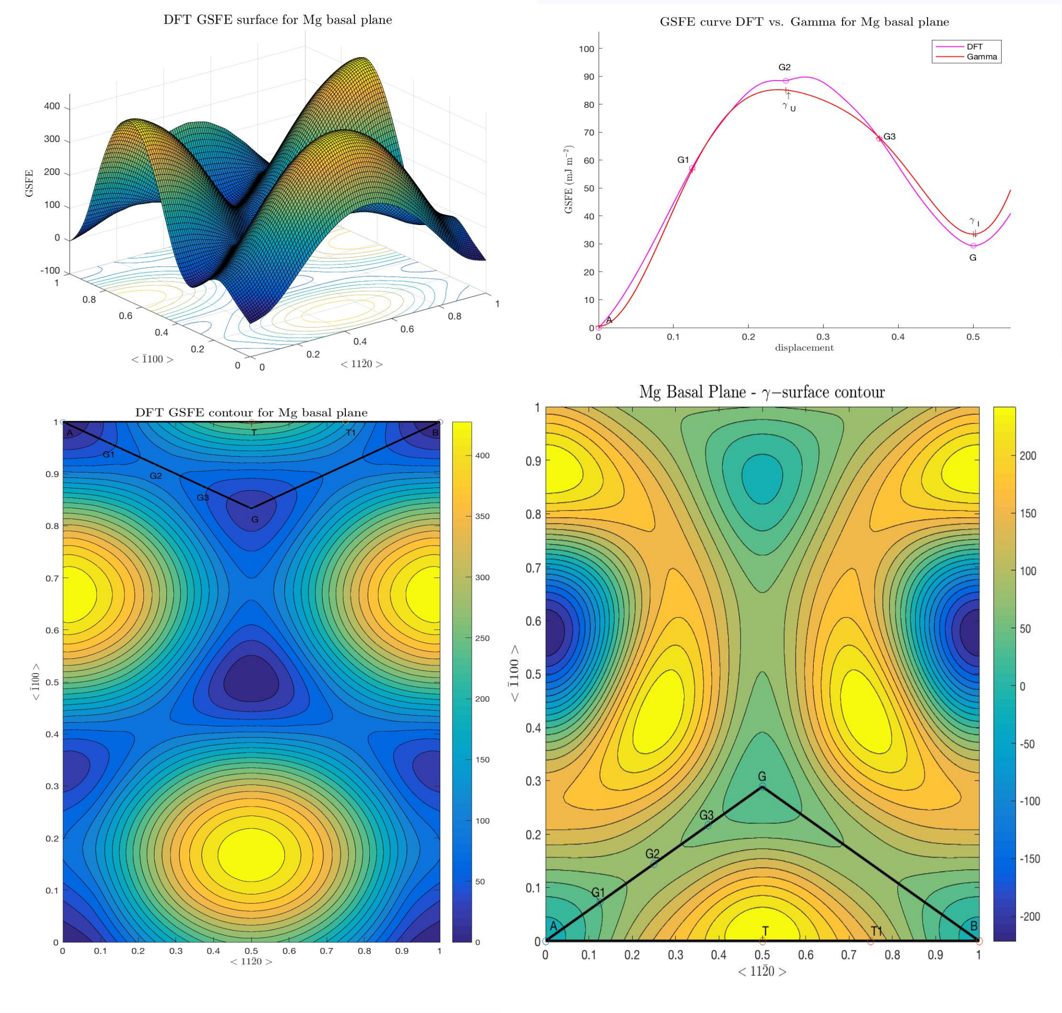
Vitek, Philo. Mag. 18, 1968

## Partial Dislocations



*Vitek and Kroupa, Generalized Splitting of Dislocations, 1968*

# Magnesium basal plane {0001} and γ-surface




**Δ**AGB: vectors for a perfect and 2 partial dislocation

**Schoeck** parameterization uses 7 GSFE values taken from the **Δ**AGB (DFT) to generate a γ-surface that can be input into the PFDD code.

$$
\begin{aligned}
\gamma[x,y] = {} & c1*(\cos(2p*y)+\cos(p*y+q*x)+\cos(p*y-q*x)) \\
& +c2*(\cos(2q*x)+\cos(3p*y+q*x)+\cos(3p*y-q*x)) \\
& +c3*(\cos(4p*y)+\cos(2p*y+2q*x)+\cos(-2p*y+2q*x)) \\
& +c4*(\cos(p*y+3q*x)+\cos(-p*y+3q*x)+\cos(4p*y+2q*x) \\
& \quad +\cos(-4p*y+2q*x)+\cos(5p*y+q*x)+\cos(5p*y-q*x)) \\
& +a1*(\sin(2p*y)-\sin(p*y+q*x)+\sin(-p*y+q*x)) \\
& +a3*(\sin(4p*y)-\sin(2p*y+2q*x)+\sin(-2p*y+2q*x))
\end{aligned}
$$

Constants:

$c0 = 0.823*(4*G-6*G1+6*G2-7.392*G3+0.804*T+0.804*T1)$

$c1 = 0.274*(-8*G+12*G1-12*G2+14.785*G3-1.608*T+0.215*T1)$

$c2 = 0.091(23.072*G-29.138*G1+32.785*G2-42.215*G3+2.569*T-2.412*T1)$

$c3 = 0.137*(-8*G+12*G1-12*G2+14.785*G3+0.215*T-1.608*T1)$

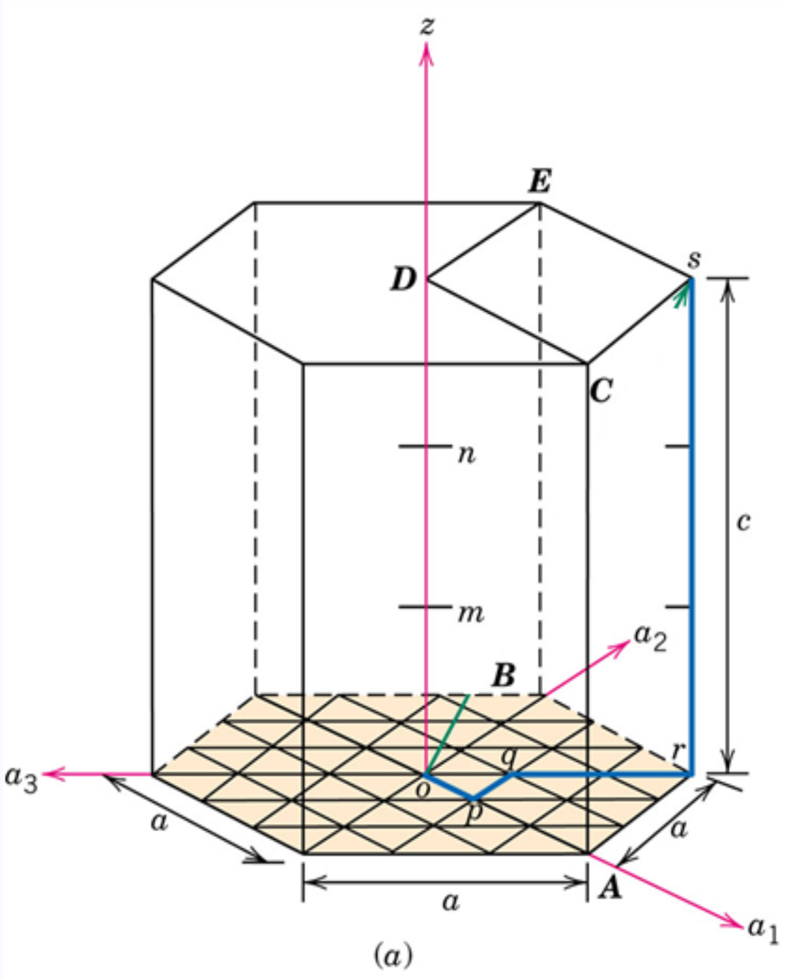
$c4 = 0.023*(1.856*G-13.723*G1+6.431*G2-4.277*G3-0.962*T+3.531*T1)$

$a1 = 0.137*(-32*G+48*G1-48*G2+62.785*G3-4.608*T-2.785*T1)$

$a3 = 0.046*(17.072*G-19.292*G1+31.923*G2-34.708*G3+3.341*T-8.354*T1)$

Schoeck, Philo. Mag. A 81, 2009

# HCP: Indices conversion & Lattice Rotation




## Indices Conversions

- Miller-Bravais $[uvtw]$
- Miller $[UVW]$

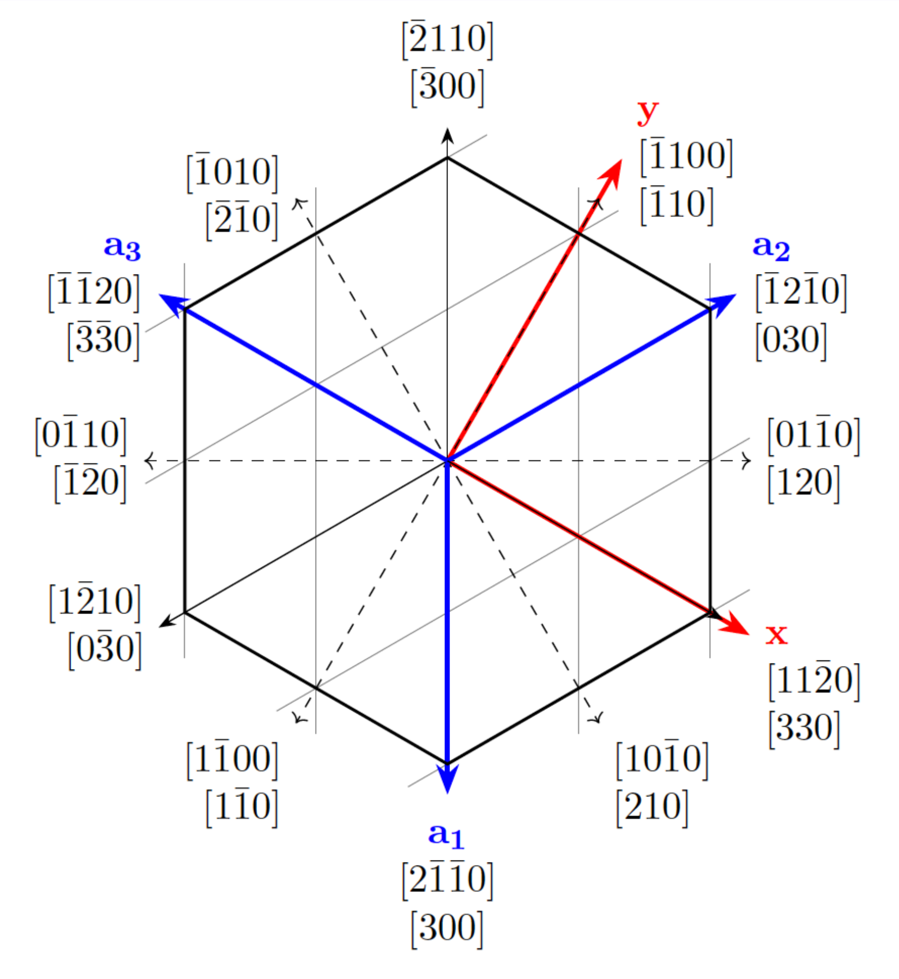
$$U = u - t$$
$$V = v - t$$
$$W = w$$

Normalize by magnitude

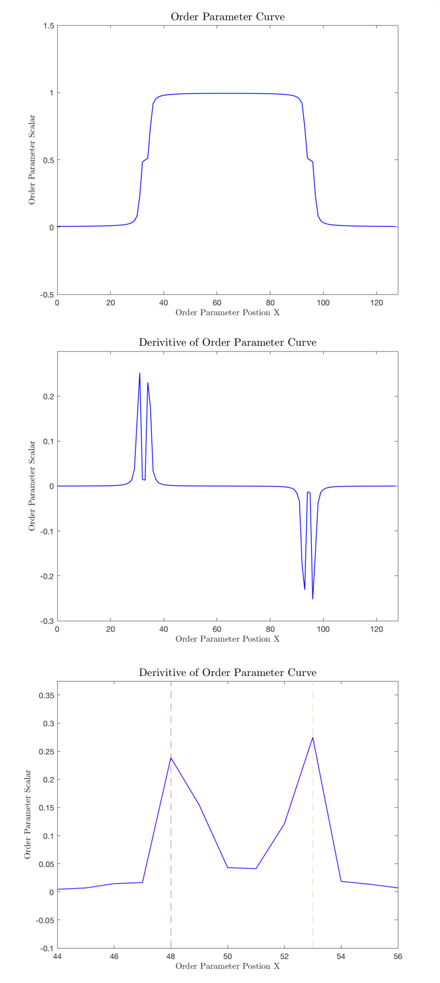
## Lattice Rotation

- x-axis: $[11\bar{2}0] \rightarrow [100]$
- y-axis: $[\bar{1}100] \rightarrow [010]$

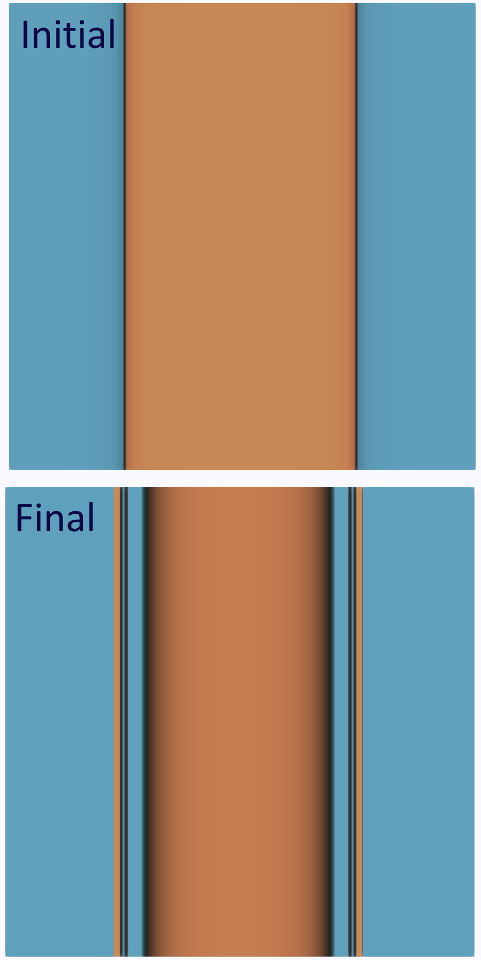
$$[R_B]_I = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{-\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

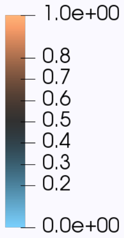


# Results

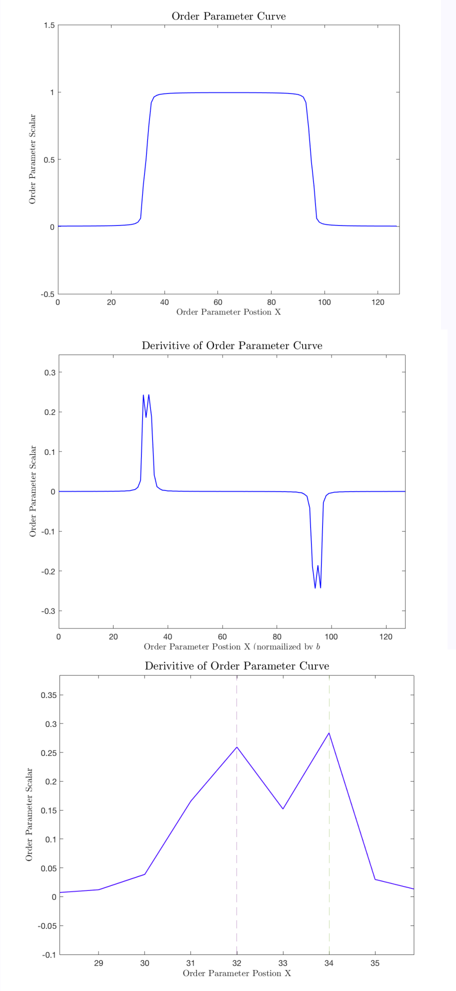



## Edge

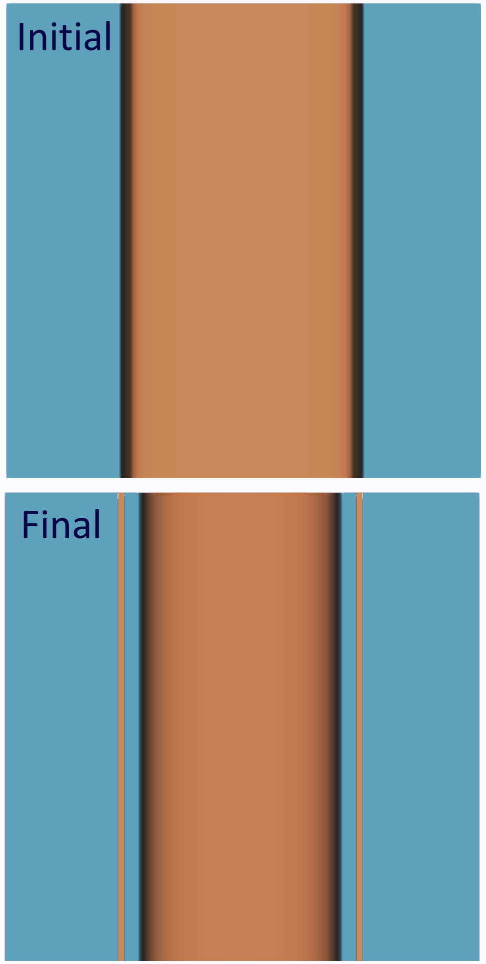


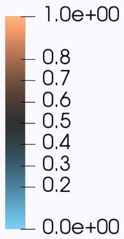




| | SFw |
|---|---|
| Edge | 5b |
| Screw | 2b |




## Screw

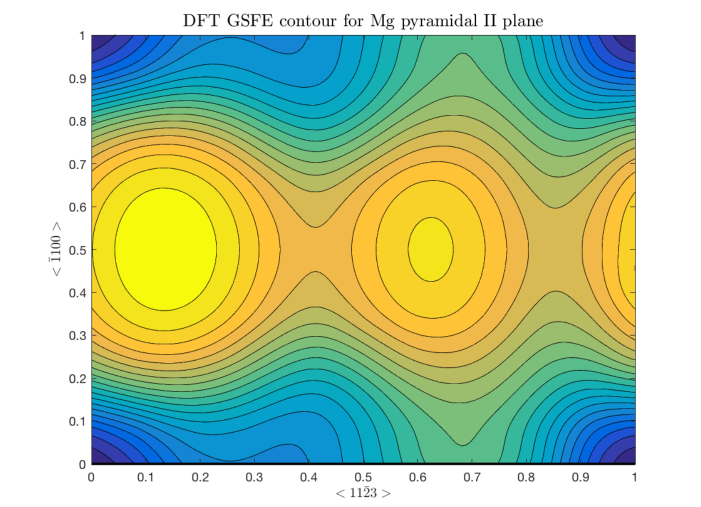


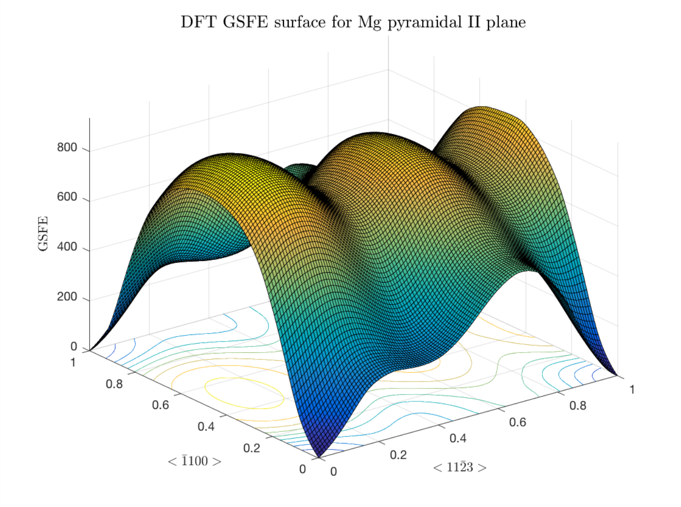



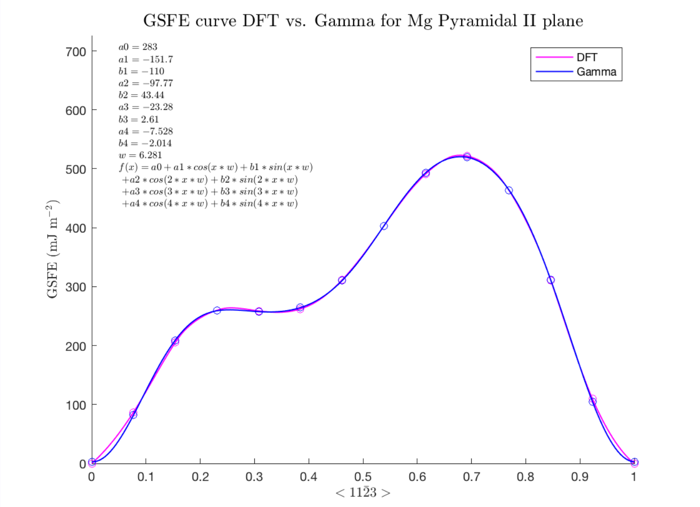
# Comparison of calculations for SF width

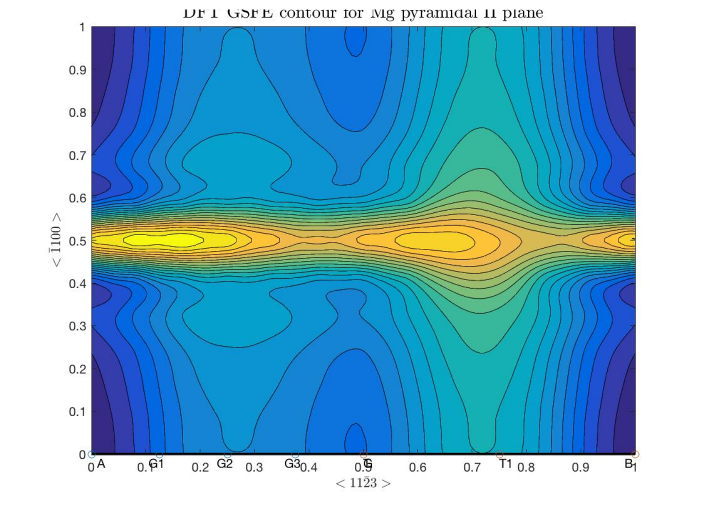
| Mg Basal Stacking Fault Widths | | | | | |
|---|---|---|---|---|---|
| Author | EDGE | SCREW | b (Å) | Method | Additional |
| **Weaver** | **5 b** | **2 b** | **3.19** | **PFDD** | **Schoeck Parameterization** |
| Yasi et al | 5.2 b | 2.0 b | 3.2 | *Ab initio* | VASP, LGF, GGA with P&W exchange-correlation potential flexible B.C. |
| | 4.5 b | 2.0 b | 3.2 | Sun EAM | periodic in dislocation line direction |
| | 4.0 b | 0.4 b | 3.2 | Liu EAM | periodic in dislocation line direction |
| Yin et al | 7.5 b | 3.5 b | 3.186 | AniLinElastTheory | Lattice/ elastic constants from experiements, SFE from DFT |
| | 7.0 b | 4.0 b | 3.189 | *Ab initio* | VASP, GGA with PBE parameterization |
| Wu et al | 2.20 b | 1.26 b | 3.187 | *Ab initio* | DFT |
| | 3.92 b | 1.26 b | 3.187 | MEAM | |
| Fan et al | 8.5 b | 4.38 b | 3.2 | Peierls-Nabarro | fits surface with reciprocal lattice vectors to a 2D Fourier series |
| Shen et al | 5.88 b | 2.16 b | ∗3.2 | EAM | |
| Groh et al | 8.0 b | 5.13 b | ∗3.2 | EAM | |
| Wang et al | 6.66 b | -- | ∗3.2 | Peierls-Nabarro | |

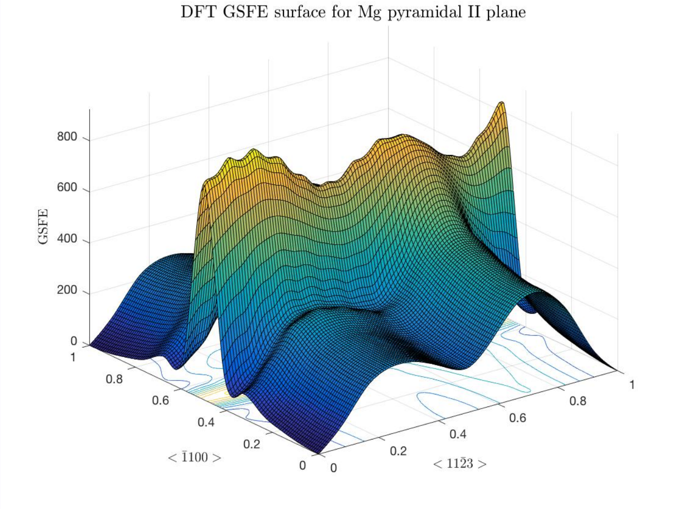
# Magnesium pyramidal II plane γ-surface

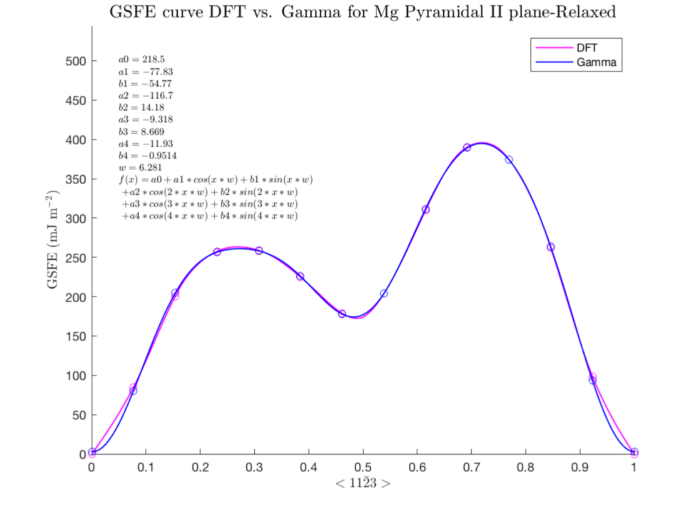


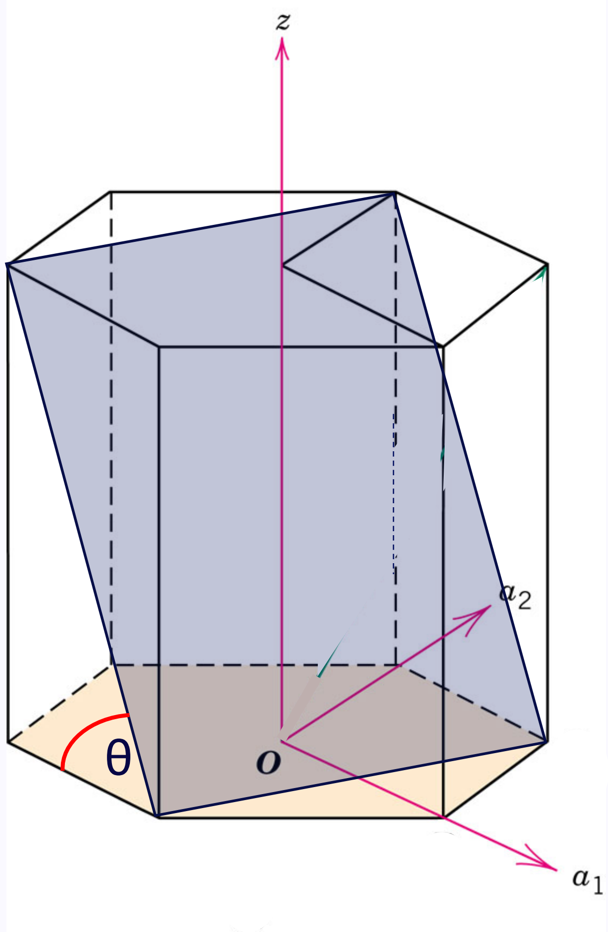



# HCP: Lattice rotation for Pyramidal II



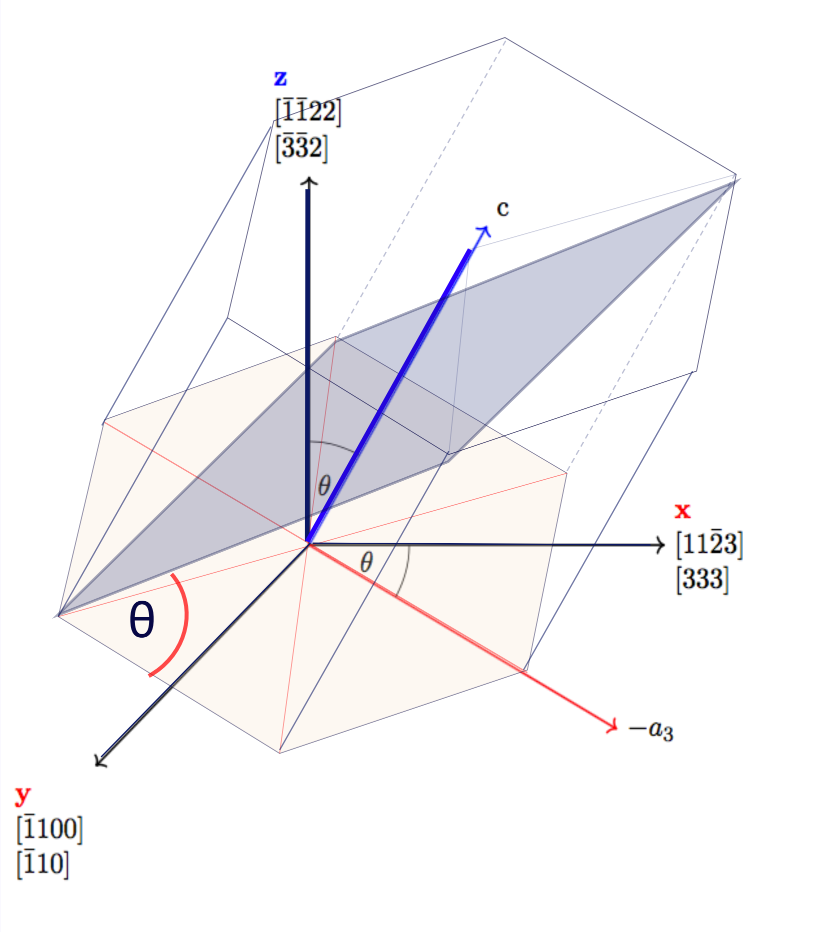

## Lattice Rotation

- x-axis: $[11\bar{2}3] \rightarrow [100]$
- y-axis: $[\bar{1}100] \rightarrow [010]$
- We can apply an additional rotation to the basal plane rotation, $[R_B]_I$, around the y axis by θ to get:

$$[R_P]_I = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix} [R_B]_I$$

$$\cos\theta = \frac{a^2}{\sqrt{a^2+c^2}} \qquad \sin\theta = \frac{c^2}{\sqrt{a^2+c^2}}$$

$$[R_P]_I = \begin{bmatrix} \frac{a}{2\sqrt{a^2+c^2}} & \frac{a}{2\sqrt{a^2+c^2}} & \frac{c}{\sqrt{a^2+c^2}} \\ \frac{-\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{c}{2\sqrt{a^2+c^2}} & -\frac{c}{2\sqrt{a^2+c^2}} & \frac{a}{\sqrt{a^2+c^2}} \end{bmatrix}$$



# Whats Next?

- Pyramidal II:
  - Add 1D fit equation to the code for preliminary results
  - Fit for the entire 2D surface and add to code
- Take a look at the Prismatic slip planes
  - Conduct a literature review of dislocation dissociation on this plane
  - Fit the gamma surface
  - Create a rotation matrix for easy input into code
- Implement for other HCP materials and Mg alloys
  - Generalize the gamma surface parameterization for each slip plane so only a few GSFE points from the surface at key points are required for the code.
- Begin to look at other microstructural influences (i.e. twinning, dislocation nucleation, etc.) on plastic deformation within HCP materials

# Material constants and Equations

**Used**

a = 3.19E-10;

b = 3.19E-10;

mu = 18.0E9;

young = 46.8E9;

c0 = 112.6205E-3;

c1 = 0.7200E-3;

c2 = -58.3781E-3;

c3 = 28.1313E-3;

c4 = -3.9212E-3;

a1 = 25.2325E-3;

a3 = -23.8545E-3;

isf = 29.3216E-3;

usf = 88.4906E-3;

**DTF Derived**

C12 = 27E9;

C11 = 63E9;

C44 = 0.5(C11-C12) = 18E9;

ll = C12 = 27E9;

mu = C44 = 0.5(C11-C12) = 18E9;

young = mu(3.0*ll+2.0*mu)/(mu+ll) = 46.8E9;

nu = young/2.0/(mu)-1.0 = 0.3;

S11 = 1.0/(young) = 2.14E-11;

S12 = -nu/(young) = -6.41E-12;

S44 = 2.0*(S11-S12) = 5.56E-11;

**Simmons&Wang**

C12 = 25.94E9;

C11 = 63.48E9;

C44 = 0.5*(C11-C12) = 18.77E9;

ll = C12 = 25.94E9;

mu = C44 = 18.77E9;

young = mu(3.0*ll+2.0*mu)/(mu+ll) = 48.43E9;

nu = young/2.0/(mu)-1.0 = 0.2901;

S11 = 1.0/(young) = 2.065E-11;

S12 = -nu/(young) = -5.990E-12;

S44 = 2.0(S11-S12) = 5.328E-11;

**Equations**

C44 = mu;

nu = young/2.0/(mu)-1.0;

C12 = 2.0*nu*C44/(1.0-2.0*nu);

C11 = 2.0*C44+C12;

ll = C12;

S11 = 1.0/(young);

S12 = -nu/(young);

S44 = 2*(S11-S12);